



A wide range of small acetylated molecules bind S3 in a variety of orientations.

A) Superimposition of the different acetylated molecules bound to site S3. The common acetyl group interaction is highlighted with dashed lines. Individual view of each of these molecules are displayed below (B-E). Acetylcholine, GalNAc, ManNAc, and CysNAc are shown in yellow, green, pink, and orange, respectively. The main polar interactions are represented by dashed red lines, with their associated distances.

